Probing the Electronic Structures of $[Cu_2(\mu\text{-}XR_2)]^{n+}$ Diamond Cores as a Function of the Bridging X Atom (X = N or P) and Charge (n = 0, 1, 2)

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Supporting Information

Figure S1 Molecular structure of $[Cu_2(PNP\text{-}2H)_2][BF_4]_2$ (anions and solvent molecules, as well as the other dication found in the asymmetric unit, are omitted).

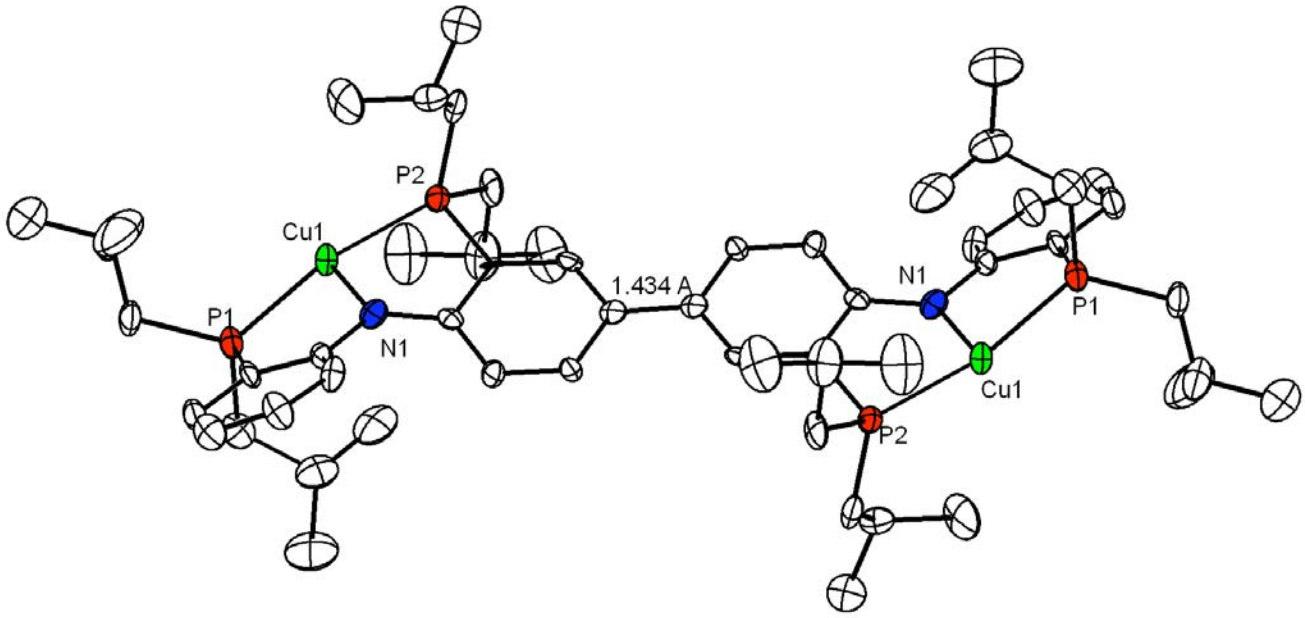


Figure S2. Fully labeled diagram of $[Cu_2(PNP\text{-}2H)_2][BF_4]_2$. For the dicationic Cu units, half of the atoms were generated by symmetry operations. See Figure S1.

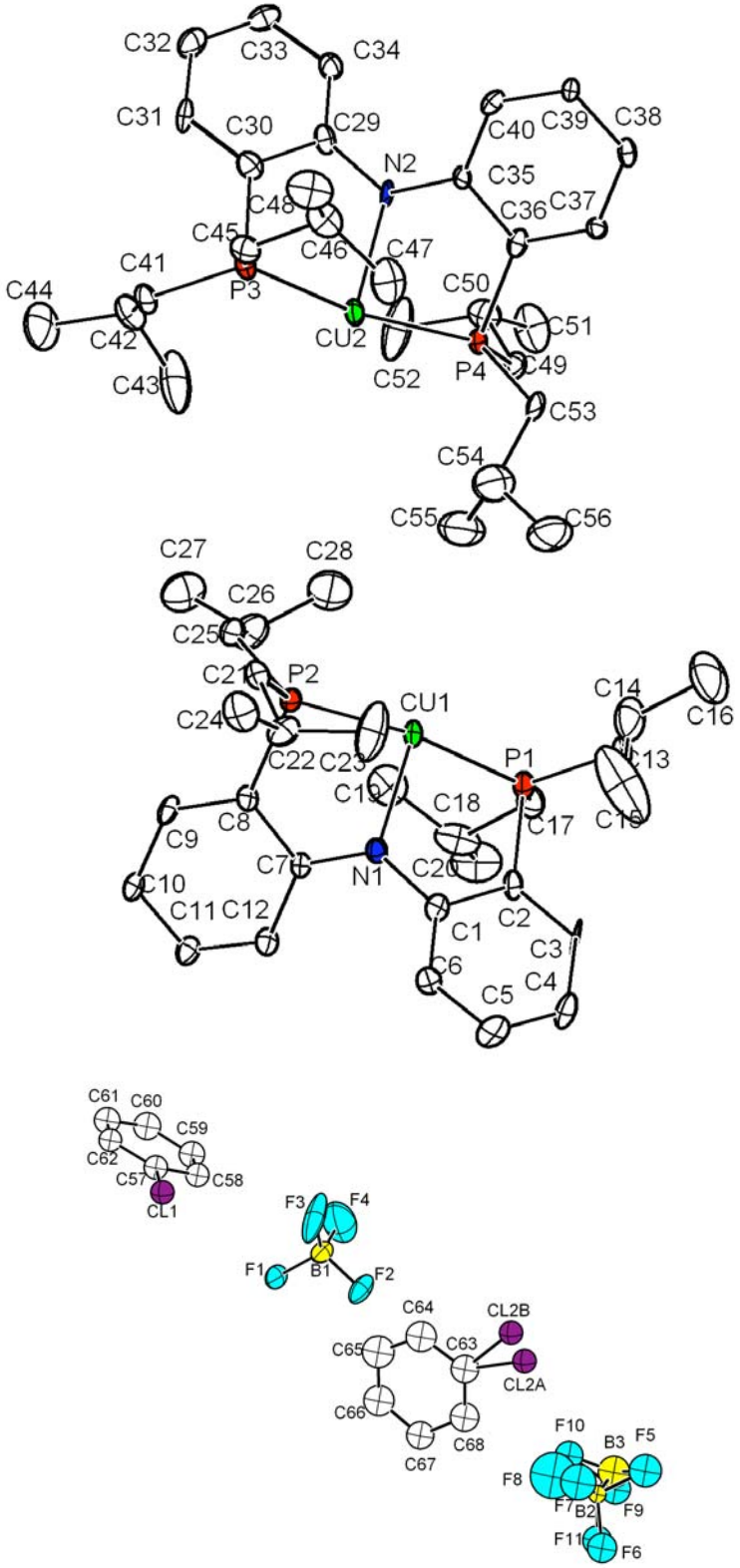
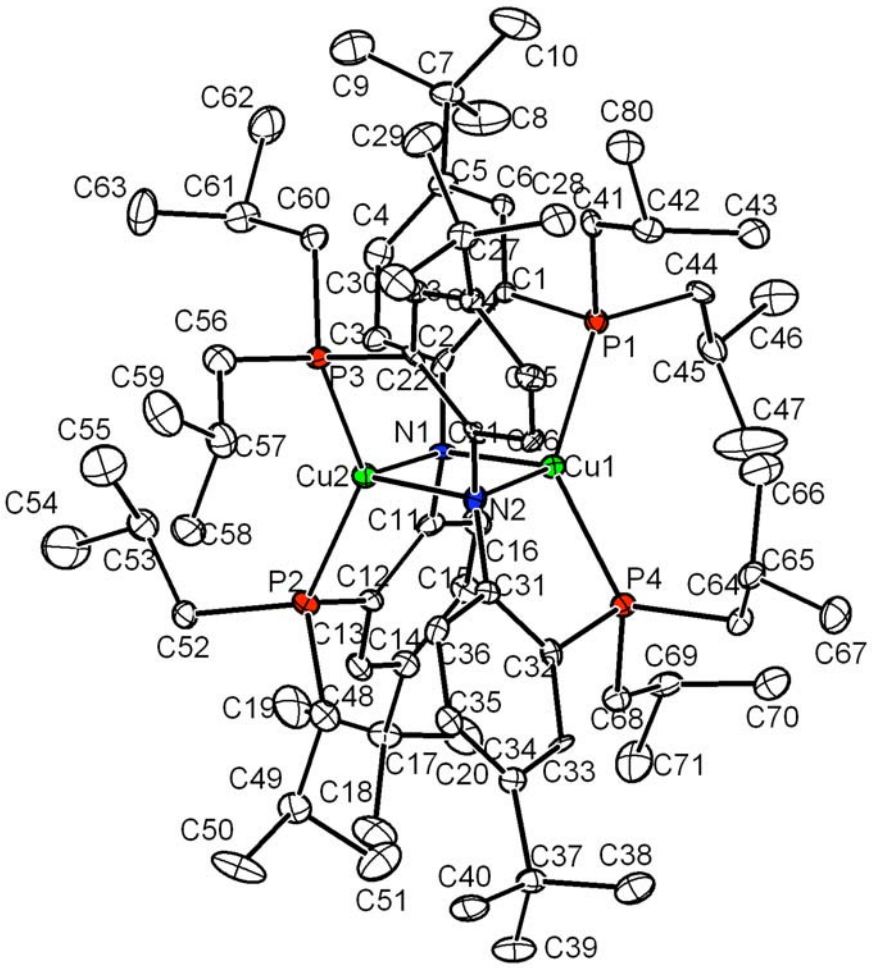
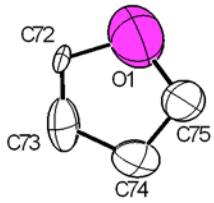


Table S1. Crystal data and structure refinement for $[Cu_2(PNP\text{-}2H)_2][BF_4]_2$.

Identification code	sbh43	
Empirical formula	$C_{68}H_{96}B_2Cl_2Cu_2F_8N_2P_4$	
Common name	$[Cu_2(PNP\text{-}2H)_2][BF_4]_2$.	
Formula weight	1436.95	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.9248(18) Å	α = 63.644(4)°.
	b = 18.516(3) Å	β = 76.885(3)°.
	c = 19.469(3) Å	γ = 71.259(3)°.
Volume	3629.5(10) $Å^3$	
Z	2	
Density (calculated)	1.315 Mg/m^3	
Absorption coefficient	0.808 mm^{-1}	
F(000)	1504	
Crystal size	.012 x .004 x .001 mm^3	
Theta range for data collection	1.81 to 28.28°.	
Index ranges	$-14 \le h \le 15$, $-24 \le k \le 23$, $-25 \le l \le 25$	
Reflections collected	19346	
Independent reflections	14697 [R(int) = 0.0631]	
Completeness to theta = 28.28°	81.6 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14697 / 20 / 738	
Goodness-of-fit on F^2	0.961	
Final R indices [I>2sigma(I)]	R1 = 0.0928, wR2 = 0.2405	
R indices (all data)	R1 = 0.1866, wR2 = 0.2980	
Largest diff. peak and hole	2.508 and -1.392 e.$Å^{-3}$	

Figure S3. Fully labeled diagram of $\{(^{t}Bu_2\text{-PNP})Cu\}_2$ (**4**).




C72
O1
C73
C75
C74

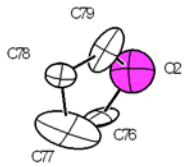

C79
C78
O2
C76
C77

Table S2. Crystal data and structure refinement for **4**.

Identification code	sbh52	
Common name	$\{(^tBu_2\text{-PNP})Cu\}_2$	
Empirical formula	$C_{72}H_{120}Cu_2N_2P_4 \cdot 2\,(C_4H_8O)$	
Formula weight	1408.87	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 23.078(2) Å	α = 90°
	b = 18.2536(18) Å	β = 94.816(2)°
	c = 19.151(2) Å	γ = 90°
Volume	8039.1(14) $Å^3$	
Z	4	
Density (calculated)	1.164 Mg/m^3	
Absorption coefficient	0.652 mm^{-1}	
F(000)	3056	
Crystal size	0.34 x 0.30 x 0.24 mm^3	
Crystal color	yellow	
Crystal habit	block	
Theta range for data collection	1.42 to 28.52°	
Index ranges	$-31 \le h \le 28$, $-23 \le k \le 23$, $-25 \le l \le 20$	
Reflections collected	49132	
Independent reflections	18310 [R_{int}= 0.1135]	
Completeness to theta = 28.52°	89.6 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	18310 / 0 / 839	
Goodness-of-fit on F^2	1.003	
Final R indices [I>2sigma(I)]	R1 = 0.0593, wR2 = 0.1012	
R indices (all data)	R1 = 0.1644, wR2 = 0.1216	
Largest diff. peak and hole	1.517 and -1.259 $e \cdot Å^{-3}$	

Figure S4. Fully labeled diagram of {(^{t}Bu$_2$-PNP)Cu}$_2$[SbF$_6$] (**5**).

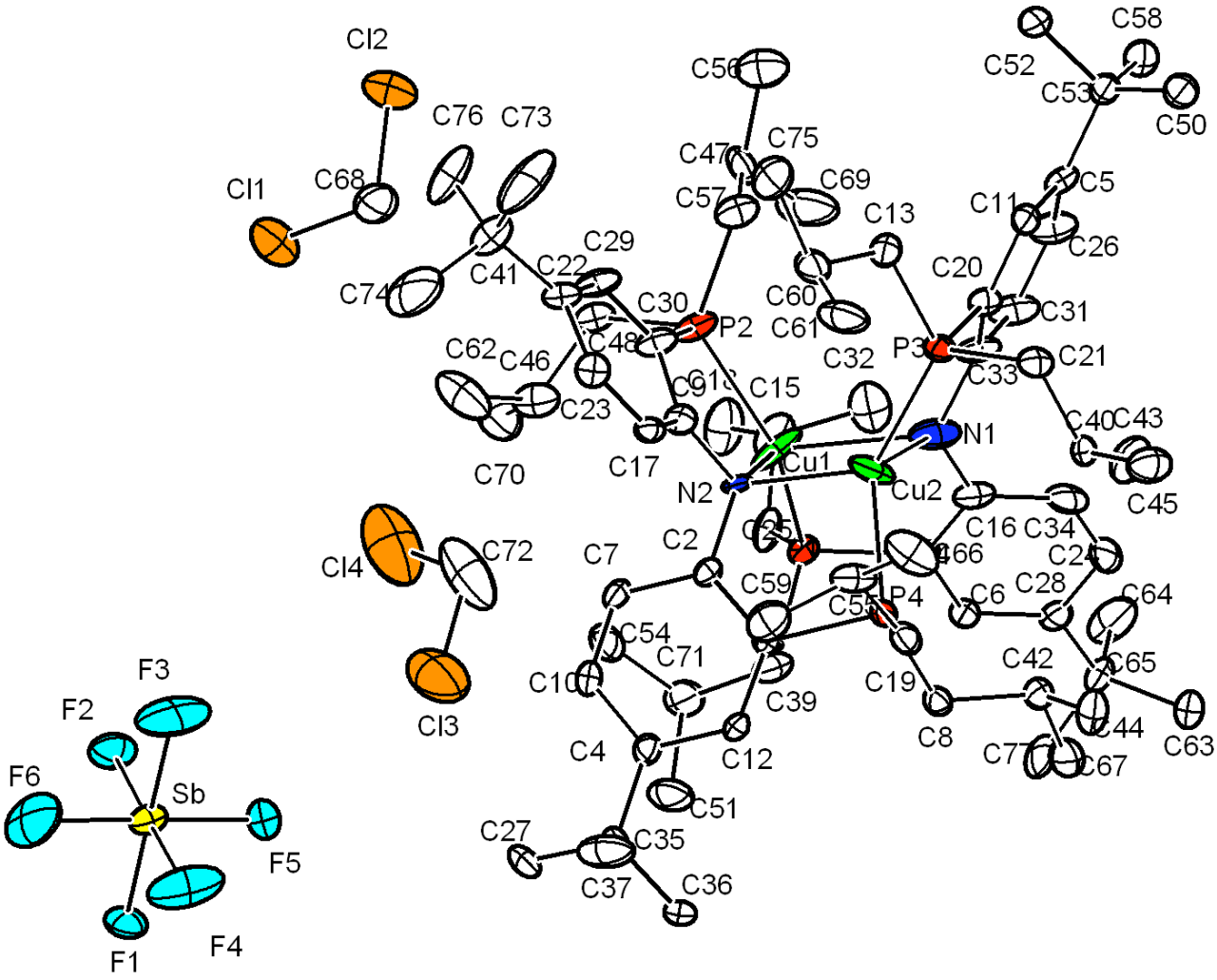


Table S3. Crystal data and structure refinement for **5**.

Identification code	sbh56	
Empirical formula	$C_{72}H_{120}ClCu_2F_6N_2P_4Sb$	
Common name	$\{(^tBu_2\text{-PNP})Cu\}_2SbF_6$	
Formula weight	1535.86	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 15.8951(8) Å	α = 90°.
	b = 14.5628(8) Å	β = 92.806(2)°.
	c = 18.0542(10) Å	γ = 90°.
Volume	4174.1(4) $Å^3$	
Z	2	
Density (calculated)	1.222 Mg/m^3	
Absorption coefficient	0.985 mm^{-1}	
F(000)	1612	
Crystal size	0.29 x 0.19 x 0.08 mm^3	
Theta range for data collection	1.75 to 38.16°.	
Index ranges	$-27 \le h \le 20$, $-20 \le k \le 22$, $-24 \le l \le 28$	
Reflections collected	50922	
Independent reflections	26121 [R(int) = 0.0527]	
Completeness to theta = 38.16°	68.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	26121 / 1 / 870	
Goodness-of-fit on F^2	1.581	
Final R indices [I>2sigma(I)]	R1 = 0.0615, wR2 = 0.0913	
R indices (all data)	R1 = 0.0915, wR2 = 0.0949	
Absolute structure parameter	0.085(10)	
Largest diff. peak and hole	3.405 and -3.759 $e.Å^{-3}$	

Figure S5. Fully labeled diagram of $\{(^{t}Bu_2\text{-PNP})Cu\}_2[SbF_6]_2$ (**6**).

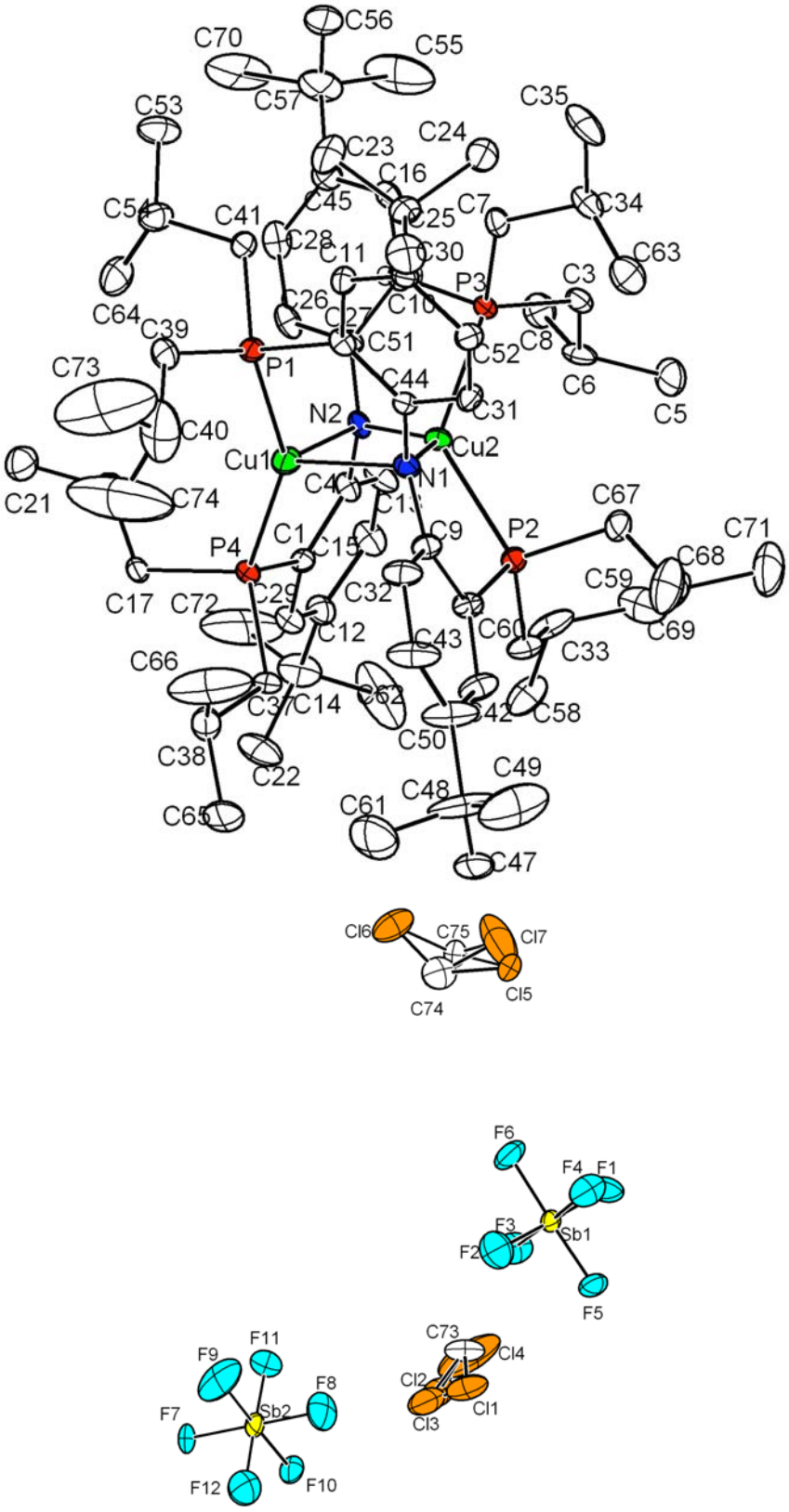


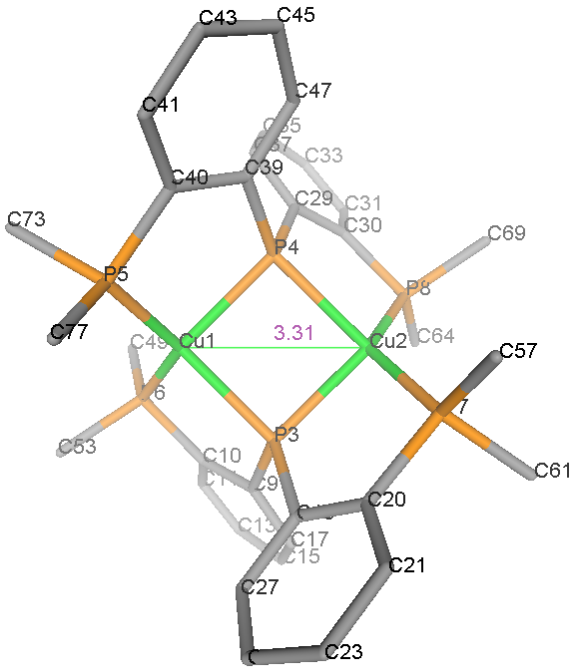
Table S4. Crystal data and structure refinement for **6**.

Identification code	sbh55sad	
Common Name	{(^{t}Bu$_2$-PNP)Cu}$_2$[SbF$_6$]$_2$, (CH$_2$Cl$_2$)	
Empirical formula	[C$_{72}$ H$_{120}$ Cu$_2$ N$_2$ P$_4$] [SbF$_6$]$_2$, (CH$_2$Cl$_2$)$_2$	
Formula weight	1906.01	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	Cc	
Unit cell dimensions	a = 19.101(3) Å	α = 90°
	b = 21.849(3) Å	β = 90.717(14)°
	c = 20.734(5) Å	γ = 90°
Volume	8653(3) Å^3	
Z	4	
Density (calculated)	1.463 Mg/m^3	
Absorption coefficient	1.365 mm^{-1}	
F(000)	3912	
Crystal size	0.31 x 0.25 x 0.22 mm^3	
Crystal color	blue	
Crystal habit	rough block	
Theta range for data collection	1.72 to 42.05°	
Index ranges	-35 ≤ h ≤ 35, -40 ≤ k ≤ 37, -38 ≤ l ≤ 38	
Reflections collected	84699	
Independent reflections	41600 [R_{int} = 0.0563]	
Completeness to theta = 42.05°	88.3 %	
Absorption correction	SADABS	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	41600 / 2 / 967	
Goodness-of-fit on F^2	1.179	
Final R indices [I>2sigma(I)]	R1 = 0.0532, wR2 = 0.0963	
R indices (all data)	R1 = 0.1041, wR2 = 0.1085	
Absolute structure parameter	-0.005(7)	
Largest diff. peak and hole	2.037 and -1.166 e·Å^{-3}	

Coordinates of simplified computational models derived from their crystal structures[1]

1: $^{1}\{(PPP)Cu\}_2^{0}$ E(BP/SDD) = -3686.09627587 a.u.
2: $^{2}\{(PPP)Cu\}_2^{+}$ E(BP/SDD) = -3685.95217995 a.u.
3: $^{1}\{(PPP)Cu\}_2^{2+}$ E(BP/SDD) = -3685.65892719 a.u.
4: $^{1}\{(PNP)Cu\}_2^{0}$ E(BP/SDD) = -3112.86073685 a.u.
5: $^{2}\{(PNP)Cu\}_2^{+}$ E(BP/SDD) = -3112.69917365 a.u.
6: $^{3}\{(PNP)Cu\}_2^{2+}$ E(BP/SDD) = -3112.38616153 a.u.

[1] Density functional calculations were carried out using the Gaussian03 suite. See experimental section of the maintext for this paper. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. J. Montgomery, T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian03, (2004) Gaussian, Inc., Pittsburgh PA.

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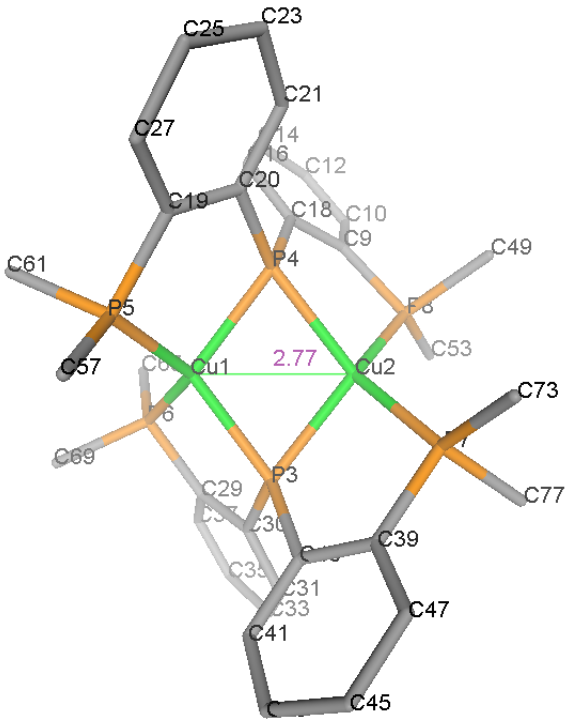

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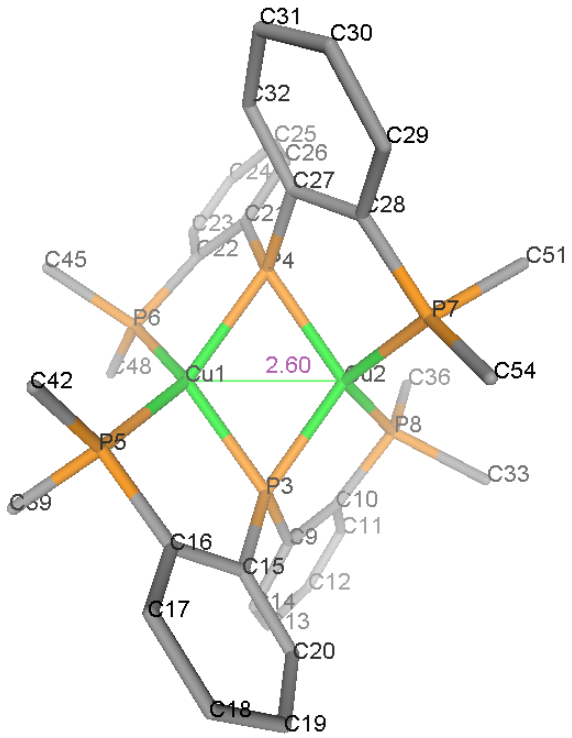


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C  0.1653  4.6601 -2.9374
C  0.3498  4.0136 -1.7144
C  0.4087  2.8425  1.4417
C  1.3437  2.3015  2.3661
C  1.4985  2.9351  3.5913
C  0.7954  4.0987  3.8863
C -0.0662  4.6642  2.9514
C -0.2479  4.0255  1.7315
C  3.8946 -1.7454 -1.1674
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H	3.6424	-2.4839	-0.4035
H	4.5049	-2.1893	-1.9567
C	2.8226	-0.0567	-3.3454
H	1.9549	0.3737	-3.8496
H	3.5901	0.6917	-3.1375
C	-3.8655	-1.9566	1.0800
H	-4.4514	-2.4362	1.8669
H	-3.5674	-2.7321	0.3714
C	-3.0087	-0.0964	3.2309
H	-3.8742	0.5255	2.9929
H	-2.2108	0.4977	3.6812
C	-3.8439	1.9887	-1.0387
H	-3.5195	2.6646	-0.2447
H	-4.4102	2.5254	-1.8028
C	-3.0861	0.1602	-3.1745
H	-3.9368	-0.4651	-2.8957
H	-2.3248	-0.4221	-3.6978
C	3.9123	1.7752	1.1718
H	3.6588	2.5687	0.4658
H	4.5207	2.2039	1.9709
C	2.9056	0.0275	3.3024
H	3.7124	-0.6788	3.0957
H	2.0808	-0.4725	3.8143
H	2.1114	-2.6782	-4.1992
H	0.9740	-4.6680	-4.5847
H	-0.3629	-5.6091	-3.0019
H	-0.8235	-4.4777	-1.0217
H	-2.0866	-2.6074	4.2017
H	-0.7566	-4.4643	4.7851
H	0.7657	-5.3345	3.2250
H	1.0105	-4.3463	1.1662
H	-2.1275	2.7013	-4.1376
H	-0.8667	4.5575	-4.7078
H	0.6568	5.4465	-3.1412
H	0.9766	4.3584	-1.0891
H	2.0943	2.5707	4.2336
H	0.9025	4.5096	4.7370
H	-0.5253	5.4735	3.1466
H	-0.8313	4.4073	1.0875
H	4.4474	-1.0352	-0.7283
H	3.2229	-0.7362	-3.9602
H	-4.4632	-1.3148	0.6009
H	-3.2973	-0.7778	3.9031
H	-4.4695	1.3272	-0.6204
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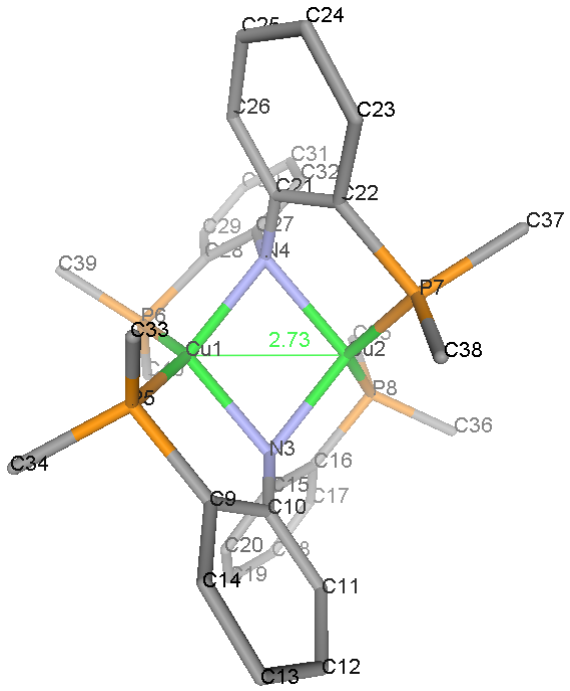
H	3.2704	0.7144	3.9309



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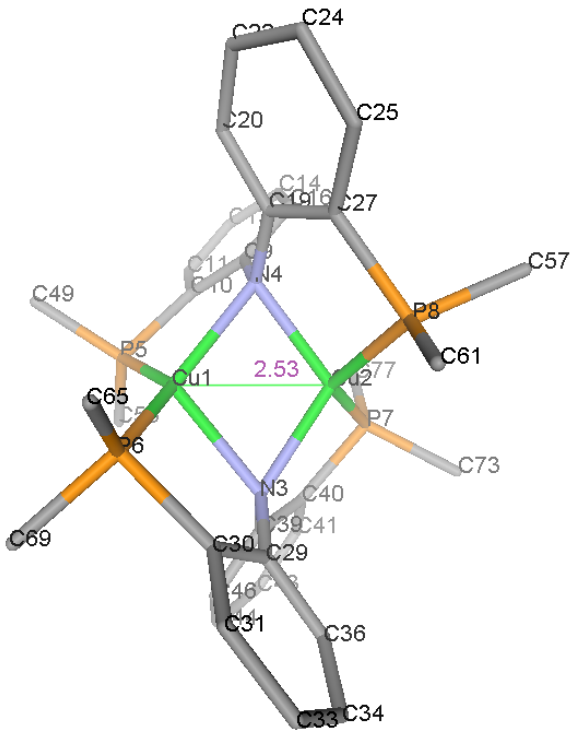
N -0.0258 1.6632 -0.0902
P -2.1441 -0.7440 1.9853
P -2.2440 0.6654 -1.9230
P 2.0860 0.8480 1.9439
P 2.1820 -0.7134 -1.9107
C -1.0055 -2.1390 2.2231
C -0.0995 -2.4456 1.1885
C 0.6975 -3.6146 1.3685
C 0.5351 -4.4363 2.4575
C -0.3932 -4.1721 3.4795
C -1.1139 -2.9979 3.3377
C 0.1388 -2.4295 -1.1631
C 1.0680 -2.1159 -2.1738
C 1.1644 -2.9721 -3.2887
C 0.3580 -4.0856 -3.4816
C -0.5801 -4.3447 -2.4854
C -0.6782 -3.5471 -1.3686
C 0.0613 2.5232 1.0321
C 0.8795 2.1959 2.1372
C 0.9310 3.0738 3.2425
C 0.2551 4.2859 3.2908
C -0.5264 4.5902 2.1698
C -0.6290 3.7363 1.0979
C -0.0902 2.3256 -1.3378
C -1.0274 1.9632 -2.3354
C -1.0552 2.6419 -3.5519
C -0.2074 3.6956 -3.8550
C 0.7300 4.0329 -2.8810
C 0.7934 3.3659 -1.6635
C -2.0043 0.1602 3.5823
C -3.7665 -1.6153 2.1770
C 2.0928 0.3978 -3.3674

C	3.8451	-1.4642	-2.1291
C	3.6400	1.8293	2.1575
C	1.9819	-0.0967	3.5228
C	-3.8027	1.6689	-2.0629
C	-2.2328	-0.3425	-3.4622
H	3.7431	2.6769	1.4767
H	-2.4664	1.1463	3.6635
H	-3.9660	-2.3985	1.4426
H	2.3820	0.0515	-4.3618
H	4.1743	-2.0772	-1.2874
H	-3.8286	2.5578	-1.4292
H	-2.8424	-1.2476	-3.5043
H	1.3575	-3.8296	0.7192
H	1.0726	-5.2181	2.5242
H	-1.7174	-2.7564	4.0313
H	-0.5505	-4.8858	4.2909
H	1.8191	-2.7765	-3.9469
H	-1.1646	-5.0885	-2.5779
H	-1.3258	-3.7636	-0.7091
H	0.5119	-4.7580	-4.3282
H	1.4577	2.8210	3.9909
H	-1.0007	5.4136	2.1495
H	-1.1926	3.9811	0.3731
H	0.4187	5.0058	4.0954
H	-1.6887	2.3703	-4.2054
H	1.3428	4.7385	-3.0551
H	1.4557	3.6221	-1.0327
H	-0.3035	4.2252	-4.8052
H	-2.3937	-0.4131	4.2885
H	-1.0419	0.2620	3.7868
H	-3.7993	-2.0189	3.0814
H	-4.4899	-0.9426	2.1246
H	1.1563	0.7144	-3.4339
H	2.6474	1.1907	-3.1641
H	3.8358	-2.0252	-2.9451
H	4.5056	-0.7402	-2.2693
H	3.6739	2.1652	3.0875
H	4.4149	1.2248	2.0286
H	2.2129	0.5170	4.2636
H	1.0402	-0.3745	3.6529
H	2.6103	-0.9850	3.6149
H	-3.9138	1.9478	-3.0063
H	-4.5713	1.0905	-1.8292
H	-2.5178	0.2438	-4.2071
H	-1.2953	-0.6048	-3.6418

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N  0.0234  1.6712 -0.2180
P -2.1537  0.4893 -1.9678
P -2.1088 -0.8517  2.0016
P  2.2407 -0.7260 -1.7970
P  1.9438  0.9617  1.9933
C -0.0093  2.2027 -1.5411
C -0.8863  1.6872 -2.5184
C -0.8822  2.2159 -3.8119
H -1.4851  1.8563 -4.4516
C -0.0345  3.2427 -4.2018
C  0.8525  3.7242 -3.2256
H  1.4652  4.4120 -3.4586
C  0.8618  3.2306 -1.9392
H  1.4700  3.5940 -1.3062
H -0.0448  3.6685 -5.2073
C  0.1117  2.6560  0.8062
C -0.5889  3.8694  0.7117
H -1.1124  4.0457 -0.0618
C -0.5327  4.8140  1.7218
H -1.0362  5.6154  1.6328
C  0.2467  4.6258  2.8700
C  0.9267  3.4148  2.9683
H  1.4468  3.2445  3.7448
C  0.8723  2.4408  1.9634
H  0.3047  5.4004  3.6376
C  0.0031 -2.4773  1.2634
C -0.8457 -2.1209  2.3246
C -0.8005 -2.8426  3.5183
H -1.3680 -2.5755  4.2309
C  0.0396 -3.9409  3.7143
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C	0.8236	-4.3158	2.6246
H	1.3809	-5.0815	2.7032
C	0.8153	-3.6142	1.4305
H	1.3684	-3.9039	0.7132
H	0.0555	-4.5323	4.6321
C	0.2222	-2.4866	-1.1122
C	1.1112	-2.1190	-2.1268
C	1.2165	-2.8960	-3.2876
H	1.8209	-2.6235	-3.9690
C	0.4708	-4.0453	-3.4790
C	-0.4186	-4.4003	-2.4574
H	-0.9489	-5.1838	-2.5543
C	-0.5426	-3.6383	-1.3122
H	-1.1645	-3.9038	-0.6442
H	0.6082	-4.6877	-4.3514
C	-3.6872	1.4784	-2.2489
H	-4.4587	0.9623	-1.9054
H	-3.8132	1.5869	-3.2261
H	-3.7049	2.4688	-1.7891
C	-2.2328	-0.7319	-3.3520
H	-1.5067	-1.3933	-3.2262
H	-2.0560	-0.2545	-4.2000
H	-3.1769	-1.2716	-3.4509
C	3.6366	1.6859	1.9678
H	4.2947	0.9515	2.0602
H	3.7384	2.2764	2.7555
H	3.8806	2.2601	1.0716
C	1.7821	0.3306	3.7141
H	0.9609	-0.2189	3.7667
H	1.6595	1.1047	4.3198
H	2.6172	-0.2661	4.0870
C	-2.3914	-0.1361	3.6718
H	-1.5145	0.1297	4.0488
H	-2.7619	-0.8431	4.2547
H	-3.0588	0.7274	3.7089
C	-3.5268	-2.1030	1.7834
H	-3.4291	-2.7965	2.4843
H	-3.4041	-2.5522	0.9099
H	-4.5527	-1.7312	1.8251
C	3.8581	-1.5729	-1.5494
H	4.5654	-0.8881	-1.4415
H	4.0721	-2.0991	-2.3595
H	3.8731	-2.2357	-0.6816
C	2.4018	0.1235	-3.4406
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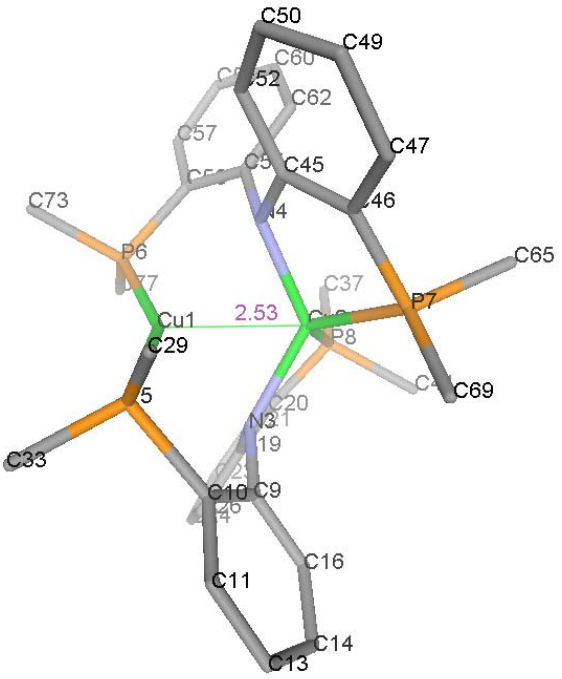
H	3.4088	0.3876	-3.7704

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N  0.2422  1.7746  0.0502
P -1.9996 -0.7569  2.0052
P -2.0040  0.9681 -1.9335
P  2.1933  0.5390  1.9052
P  1.9793 -0.6844 -1.9996
C  0.0026 -2.5427  1.1737
C -0.8503 -2.1685  2.2134
C -0.9227 -2.9585  3.3812
H -1.5056 -2.6910  4.0823
C -0.1752 -4.1051  3.5391
C  0.6998 -4.4608  2.4929
H  1.2400 -5.2377  2.5812
C  0.7892 -3.6962  1.3392
H  1.3915 -3.9564  0.6512
H -0.2519 -4.7429  4.4222
C  0.1349 -2.5261 -1.2154
C  0.8373 -2.0471 -2.3436
C  0.7074 -2.6958 -3.5730
H  1.1457 -2.3431 -4.3375
C -0.0584 -3.8568 -3.6965
C -0.6682 -4.3714 -2.5598
H -1.1526 -5.1844 -2.6242
C -0.5870 -3.7263 -1.3335
H -1.0199 -4.0964 -0.5734
H -0.1606 -4.3984 -4.6391
C -1.7395  0.2473  3.5312
H -1.4864 -0.3656  4.2664
H -0.9742  0.8555  3.3754
H -2.5899  0.8459  3.8643
C -3.6324 -1.5365  2.3080
H -3.6172 -1.9447  3.2109
```

```
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H -3.9441 -2.3007  1.5929
C  2.2325  0.1539 -3.6143
H  2.7247 -0.4638 -4.2108
H  1.3460  0.3129 -4.0212
H  2.7710  1.1034 -3.5854
C  3.5414 -1.5256 -1.4937
H  4.2233 -0.8256 -1.3428
H  3.3772 -1.9652 -0.6229
H  3.9724 -2.2710 -2.1653
C  0.3862  2.5021  1.2504
C  1.1920  2.0075  2.2980
C  1.2908  2.7228  3.4995
H  1.8532  2.3892  4.1897
C  0.5893  3.9122  3.7169
C -0.2239  4.3634  2.6854
H -0.7371  5.1532  2.8166
C -0.3122  3.6992  1.4696
H -0.8536  4.0609  0.7770
H  0.7580  4.4877  4.6295
C  0.1442  2.5948 -1.1189
C -0.7815  2.3022 -2.1434
C -0.8746  3.1598 -3.2469
H -1.5123  2.9646 -3.9225
C -0.0722  4.2838 -3.3938
C  0.8920  4.5161 -2.3916
H  1.4907  5.2466 -2.4866
C  0.9882  3.7087 -1.2721
H  1.6300  3.9069 -0.6027
H -0.2231  5.0103 -4.1950
C  3.8981  1.1944  1.6631
H  4.2073  1.5754  2.5230
H  4.4921  0.4320  1.4479
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C  2.2889 -0.4465  3.4644
H  2.1288  0.1639  4.2260
H  1.5539 -1.1089  3.4563
H  3.2257 -0.9778  3.6448
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H -3.7191  2.3917 -2.6753
H -4.3372  1.2129 -1.7892
H -3.6709  2.5494 -0.9891
C -2.0390  0.1903 -3.6042
H -1.9267  0.9066 -4.2808
H -1.2571 -0.4117 -3.6807
H -2.9344 -0.3803 -3.8597
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